Ising-Model, Block-Spin Distributions by the Markov Property Method

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The idea that, near the critical point, each block of spins behaves just like a single, big spin is investigated. The case where a diamond-shaped block of spins is embedded in a (small) sea of spins is studied. Use is made of the Markov property method to make exact computations of the various spin moments needed to test this hypothesis. The residual fluctuation about the mean value of the block spin is seen to tend to a finite fraction of the length of the mean block-spin. This result is in line with previous studies which used different types of boundary conditions.

KEY WORDS: Scaling, Ising model, Markov property, critical phenomena, parallel computational procedures.

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1. INTRODUCTION AND SUMMARY

The pioneering paper of Kadanoff[1] contained the fruitful scaling idea that near the critical point, a block of spins behaves just like one big spin. The aim of this paper is to investigate this idea by *exact calculation* for smaller size systems. Since the blocks that Kadanoff was speaking about were embedded in a sea of other spins, interacting with their neighbors and at the same temperature, we will try to model this effect as well in our calculations. To this end we will embed a diamond shaped region entirely within a square with periodic boundary conditions. This diamond-shaped, embedded feature along with the use of exact calculations make, I believe, this study distinct from previous studies of block spin distributions. Examples are the work of Binder[2], Bruce[3], and Nicolaides and Bruce[4]. Both free and periodic boundary conditions were used in these studies. The general features which emerge closely correspond to those reported in previous studies.

In the second section we outline the methods of calculation that we have used. These methods permit us to perform in modest amounts of time on a work station computations which would have taken trillions of years to do by direct methods on a tera-flop machine. This paper reports another example of the type of calculations which can be done efficiently by the Markov property method. In the third section we report our results. They are analyzed in terms of the low-order moments and in terms of the parameters of a double Gaussian distribution of the mean block spin as a function of inverse temperature. We find that at the critical point (as expected) that the mean-block spin is on the scale of $L^{\frac{7}{8}}$. The block spins are rather like a big spin, but with a dispersion in length of about 23% of their mean length.

2. MARKOV PROPERTY METHOD

A large class of important problems possess a key mathematical property called the Markov property. This property permits the introduction of new, specifically massively parallel, methods to compute the solutions. Here I sketch briefly the Markov property method. Greater detail can be found in the references[5],[6]. The Markov property is simply stated. Consider a region $\mathscr{R}$ interior to a domain $\mathscr{D}$ over which a problem is stated. Let the problem variables on the boundary $\partial\mathscr{R}$ of $\mathscr{R}$ $[\partial\mathscr{R} \cap \mathscr{R} = \emptyset\ ]$ be fixed. This statement is meant to include values, and where appropriate, derivatives *etc.* Then the problem is said to possess the Markov property, if any expectation value of problem variables supported only in $\mathscr{R}$ is independent of all the problem variables supported in $\mathscr{D} \setminus (\mathscr{R} \cup \partial\mathscr{R})$. In the simple case of the one-dimensional Ising model, this definition means that if we fix the values of spins σ_i and σ_j, where $i < j$ so that we can define, $(\partial\mathscr{R} = \{i,\ j\})$, $\mathscr{R} = \{k \mid i < k < j\}$, $\mathscr{D} = \{k \mid 1 \le k \le n\}$, then the partition function for this model becomes,

$$
\begin{aligned}
Z(\sigma_i, \sigma_j) &= \sum_{\substack{\sigma_k = \pm 1 \\ 1 \le k \le n \\ k \ne i,\, j}} \exp\left[K \sum_{k=1}^{n} \sigma_k \sigma_{k+1}\right] \\
&= \left(\sum_{\substack{\sigma_k = \pm 1 \\ k \in \mathscr{D} \setminus (\mathscr{R} \cup \partial\mathscr{R})}} \exp\left[K\sigma_j\sigma_{j+1} + K \sum_{k \in \mathscr{D} \setminus (\mathscr{R} \cup \partial\mathscr{R})}^{n} \sigma_k \sigma_{k+1}\right]\right) \\
&\quad \times \left(\sum_{\substack{\sigma_k = \pm 1 \\ k \in \mathscr{R}}} \exp\left[K\sigma_i\sigma_{i+1} + K \sum_{k \in \mathscr{R}} \sigma_k \sigma_{k+1}\right]\right) .
\end{aligned} \tag{2.1}
$$

In the case of periodic boundary conditions, we set $\sigma_{n+1} = \sigma_1$ and for free boundary conditions we set $\sigma_{n+1} = 0$. From the factorization of the partition function in (2.1) it is clear that the expectation value of any combination of spin variables supported in $\mathscr{R}$ depends only on the second factor and not at all on the first factor, since we are holding σ_i and σ_j fixed.

In order to use this property to our advantage, it is convenient to introduce a block decomposition formalism. Now we introduce the block spin sums,

$$S_\nu = \sum_{\vec{\imath} \in \mathscr{B}_\nu} w(\nu, \vec{\imath}) \sigma_{\vec{\imath}}, \tag{2.2}$$

where $\mathscr{B}_\nu$ is the portion of the space lattice which comprises block ν, and $w(\nu, \vec{\imath})$ is the fraction of site $\vec{\imath}$ in block ν and is subject to the constraints,

$$\sum_\nu w(\nu, \vec{\imath}) = 1, \quad \forall \vec{\imath}. \tag{2.3}$$

It follows immediately from (2.3) that $w = 1$ for any interior spin. Normally in, for example, two dimensions, $w = \frac{1}{2}$ for a spin on an edge, and $w = \frac{1}{4}$ or even $\frac{3}{4}$ for a corner spin on the square lattice. It could also be $w = \frac{1}{6}$ or $\frac{1}{3}$ or even $\frac{2}{3}$ or $\frac{5}{6}$ for a corner spin on a triangular lattice. We will now divide the sites on the lattice into those sites which are interior to some block, and the rest which we will call boundary spins and which set we will denote by $\mathscr{B}$. It is necessary in this decomposition that no interior spin of one block be a nearest neighbor on the lattice to an interior spin of any other block. By (2.2) and property (2.3), We can write,

$$\sum_{\vec{\imath} \in \mathscr{L}} \sigma_{\vec{\imath}} = \sum_\nu S_\nu. \tag{2.4}$$

If we next define $\langle\ \rangle_{\mathscr{C}_\nu}$ as the constrained expectation value with respect to the weight function

$$[Z(K,H)]^{-1} \exp\left(K \sum_{\vec{\imath} \in \mathscr{D}} \sum_{\vec{\delta} \in \mathscr{N}} \sigma_{\vec{\imath}} \sigma_{\vec{\imath}+\vec{\delta}} + H \sum_{\vec{\imath} \in \mathscr{D}} \sigma_{\vec{\imath}}\right) \prod_{\vec{\imath} \in \mathscr{D}} [f(\sigma_{\vec{\imath}})\, d\sigma_{\vec{\imath}}], \tag{2.5}$$

within the νth block, with all the boundary spins fixed. The set $\mathscr{N}$ is $\frac{1}{2}$ the nearest neighbor set. We further define $\langle\ \rangle_{\mathscr{B}}$ to be the expectation with respect to the boundary spins. With this notation, we can write,

$$M = |\mathscr{L}|^{-1} \sum_{\vec{\imath}\in\mathscr{L}} \langle \sigma_{\vec{\imath}} \rangle = |\mathscr{L}|^{-1} \left\langle \sum_{\nu} \left[\langle S_\nu \rangle_{\mathscr{C}_\nu} \prod_{\substack{\mu \\ \mu\neq\nu}} \langle 1 \rangle_{\mathscr{C}_\mu} \right] \right\rangle_{\mathscr{B}}$$

$$= |\mathscr{L}|^{-1} \left\langle \left(\sum_{\nu} \frac{\langle S_\nu \rangle_{\mathscr{C}_\nu}}{\langle 1 \rangle_{\mathscr{C}_\nu}} \right) \prod_{\mu} \langle 1 \rangle_{\mathscr{C}_\mu} \right\rangle_{\mathscr{B}} \qquad (2.6)$$

We observe that (2.6) has the form of a new quantity,

$$[S_\nu] \equiv \frac{\langle S_\nu \rangle_{\mathscr{C}_\nu}}{\langle 1 \rangle_{\mathscr{C}_\nu}} \qquad (2.7)$$

which depends only on the boundary spins of $\mathscr{B}_\nu$, which set we denote as $\partial\mathscr{B}_\nu$, whose expectation value we are taking, with respect to all the boundary spins, $\mathscr{B} = \cup_\nu \partial\mathscr{B}_\nu$, by the use of an additional weighting factor,

$$\prod_{\mu} \langle 1 \rangle_{\mathscr{C}_\mu}, \qquad (2.8)$$

as displayed by (2.6).

The rest of the quantities that we will be needing can be explicitly expressed in terms of the block quantities. As an illustration considered the susceptibility,

$$\chi(k) = |\mathscr{L}|^{-1} \sum_{\vec{\imath}\in\mathscr{L}} \sum_{\vec{\jmath}\in\mathscr{L}} \langle \sigma_{\vec{\imath}} \sigma_{\vec{\jmath}} \rangle = |\mathscr{L}|^{-1} \left\langle \sum_{\nu} \sum_{\mu} S_\nu S_\mu \right\rangle$$

$$= |\mathscr{L}|^{-1} \left\langle (T_2 - T_3 + T_1^2) \prod_{\lambda} \langle 1 \rangle_{\mathscr{C}_\lambda} \right\rangle_{\mathscr{B}}, \qquad (2.9)$$

where

$$T_1 = \sum_{\nu} [S_\nu], \quad T_2 = \sum_{\nu} [S_\nu^2], \quad T_3 = \sum_{\nu} [S_\nu]^2. \qquad (2.10)$$

Further details are given in reference (6).

The *modus operandi* is to start with small 2×2 and 3×3 diamonds and join them together by summing over the boundary spins which are

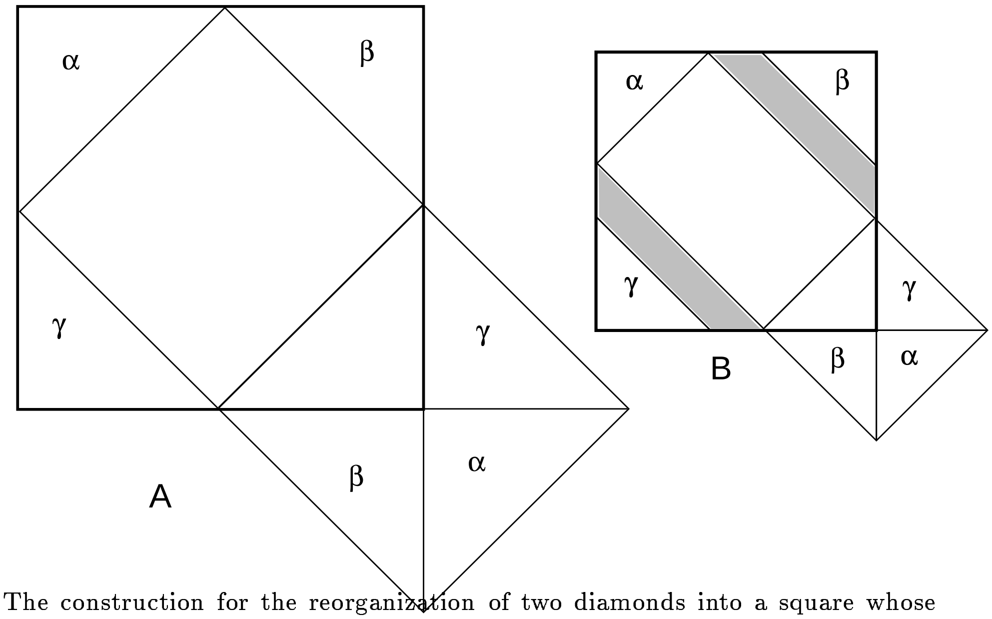

Fig. 1. The construction for the reorganization of two diamonds into a square whose edge is equal the the tip-to-tip width of the diamonds. A is for squares whose edge length is even and B is for odd squares. The trapezoidal bridges are the shaded areas.

common to two or more of the small diamonds to produce the results for the larger diamond as a function of the boundary spins. In this way for the two-dimensional square lattice, results have been obtained up through the 6×6 diamond. It is possible for the case of periodic boundary conditions, as shown in Figure 1, to join two diamonds together to get a square. For squares whose edge length is even, the construction is shown in Fig. 1 A. For squares whose edge length is odd, the construction is shown in Fig. 1 B. Here we use an $(n+1) \times (n+2)$ rectangle, an $(n+1)$-diamond and two trapezoidal bridges of unit thickness and edges $(n+1)$ and $(n+2)$ to form a $(2n+1) \times (2n+1)$ square. These bridges have no internal spin sums to be done. The method we will employ in this study is to study the behavior of one of these two diamonds, which gives us a diamond shaped block embedded in a (small) sea of spins.

3. BLOCK SPIN ANALYSIS

Baker and Krinsky[7] and Newman[8] have proven rigorously that the distribution of the mean block-spin is a Gaussian centered on zero in the high temperature region and is the sum of two Gaussians centered on plus or minus the spontaneous magnetization in the low temperature region in the limit of infinite block size. The dispersion is given by the magnetic susceptibility. These mean block-spins are independent of each other in the limit of infinite block size, but this feature has not been established at the critical point. We will examine the behavior of the block spin distribution by fitting the low order moments to the sum of two Gaussian distributions. This form is rigorously correct both above and below the critical point, as we have just remarked, for infinite block size. From the studies[2–4] on blocks, this form is reasonable (if not quite perfect) at the critical point as well. Thus we will use the following form for our present purposes.

$$f(x) = \frac{1}{2\sigma\sqrt{2\pi}}\left[\exp\left(-\frac{(x-\delta)^2}{2\sigma^2}\right) + \exp\left(-\frac{(x+\delta)^2}{2\sigma^2}\right)\right] \tag{3.1}$$

It is simple to compute for this distribution that

$$\langle x^2\rangle = \delta^2+\sigma^2, \quad \langle x^4\rangle = 3\sigma^4+6\delta^2\sigma^2+\delta^4, \quad \langle x^4\rangle - \langle x^2\rangle^2 = 2\sigma^2(\sigma^2+2\delta^2)$$

$$\delta^2 = \sqrt{\frac{3}{2}\langle x^2\rangle^2 - \frac{1}{2}\langle x^4\rangle} \qquad \sigma^2 = \langle x^2\rangle - \delta^2 \tag{3.2}$$

We have computed for a number of temperatures in the range $0 \leq K \leq K_c$ for $L \times L$ regions with periodic boundary conditions of the two-dimensional, square lattice the results for an embedded diamond shaped region of the spin-$\frac{1}{2}$ Ising model. For this model $K_c = \mathrm{arctanh}(\sqrt{2}-1) \approx 0.44068678$. The effective number of spins are 2, 8, 18, 32, and 50 in the embedded diamonds in the squares with edges 2, 4, 6, 8 and 10 respectively. That is to say, exactly half the total number of spins. The counting here

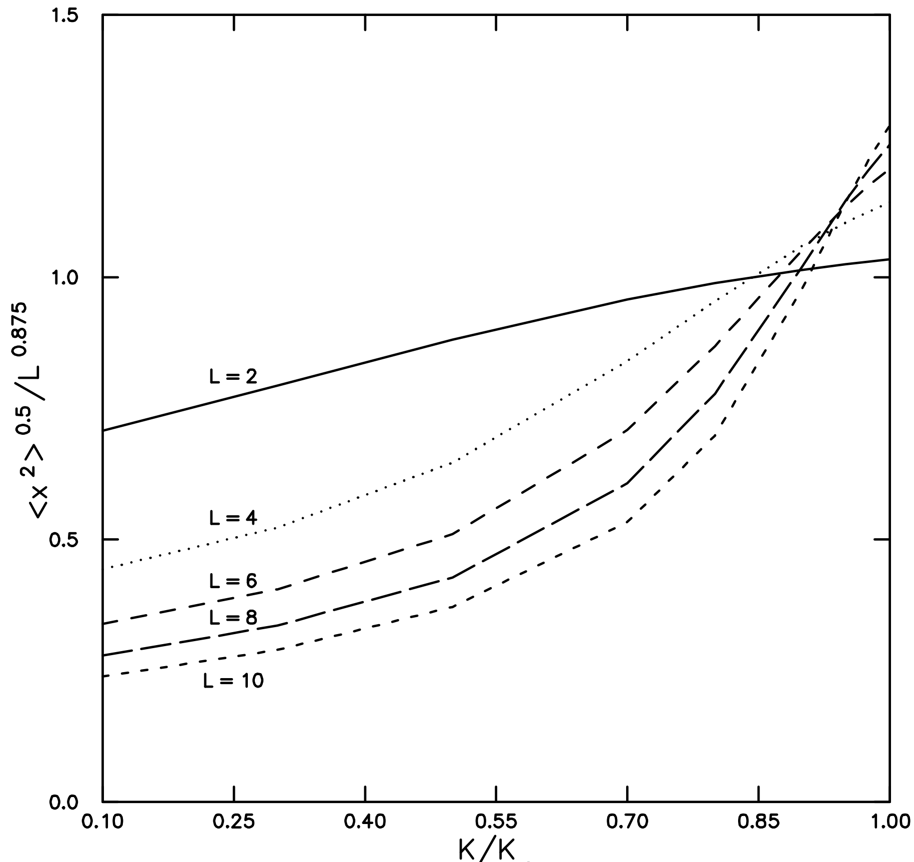

Fig. 2. The normalized root mean square spin for the embedded diamond versus the inverse temperature.

for edge and vertex spins is as in section 2. According to finite-size scaling theory,[9] the root mean square spin should scale proportionally to $L^{0.875}$ for this model as the critical index for the susceptibility is $\gamma = \frac{7}{4}$. Thus we have plotted in Fig. 2 the quantity

$$s = \langle x^2 \rangle^{\frac{1}{2}} / L^{\frac{7}{8}}. \tag{3.3}$$

It is to be observed that s appears to be tending to zero as is expected in the high temperature region (small K region), but is tending to a finite limit at the critical temperature.

The dispersion of the mean square spin is given by (3.2) in terms of

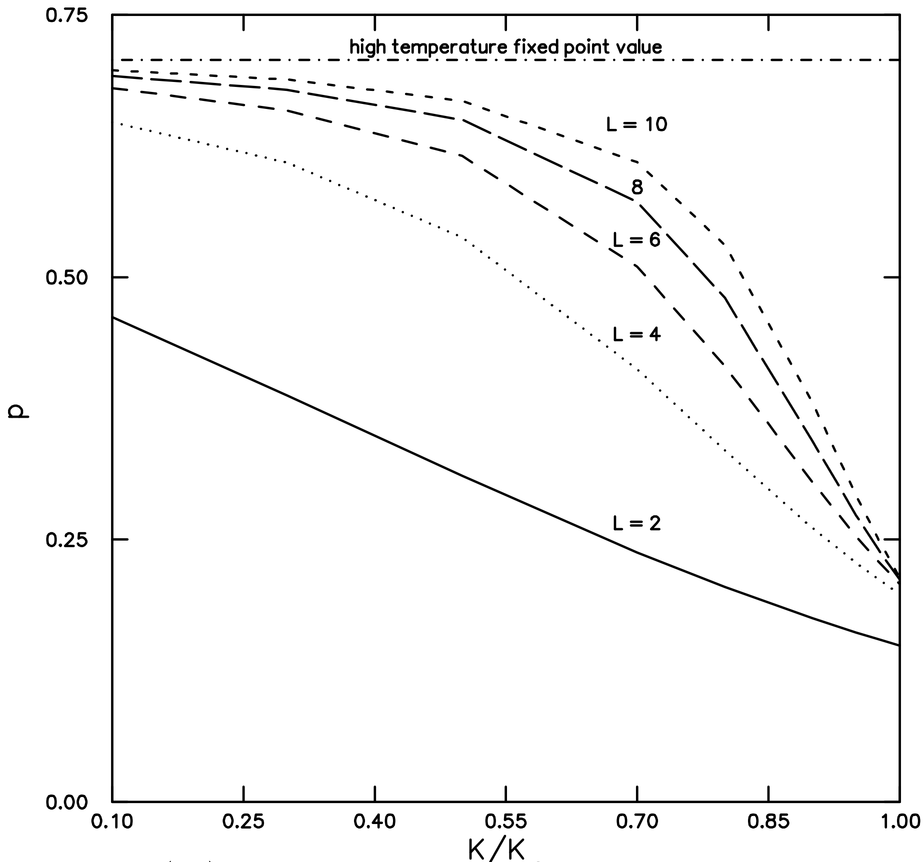

Fig. 3. The dispersion p (3.4) of the mean square spin for the embedded diamond as a fraction of the mean square spin versus the inverse temperature.

the double Gaussian parameters. Thus we plot in Fig. 3.

$$p = \frac{\sqrt{\langle x^4 \rangle - \langle x^2 \rangle^2}}{2\langle x^2 \rangle} = \frac{\sqrt{2\sigma^2(\sigma^2 + 2\delta^2)}}{2(\sigma^2 + \delta^2)} \tag{3.4}$$

It is to be noticed that for $K < K_c$ the values are tending monotonically upward with increasing L and are less than the expected high-temperature fixed point value, $1/\sqrt{2}$. At the value $K = K_c$, the limiting value is much smaller. At the critical point power law behavior in terms of the system size is typical. For example, $\chi(K_c, L) \propto L^{\frac{7}{4}}$. Reference (6) points out that for the ratio of two divergent quantities, a power-law approach to the infinite limit is to be expected. Extrapolation of p against $L^{-\frac{7}{4}}$ produces a rather

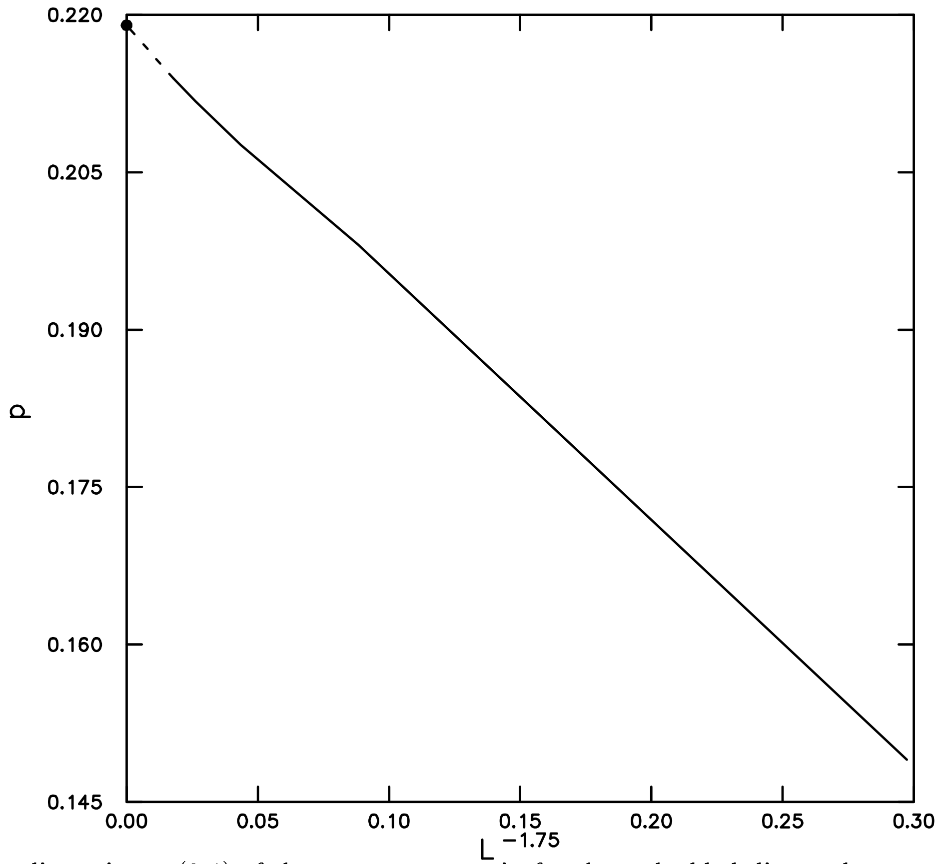

Fig. 4. The dispersion p (3.4) of the mean square spin for the embedded diamond as a fraction of the mean square spin at the critical temperature. It is plotted against $L^{-1.75}$

straight line and suggests that the limiting value is about 0.219 ± 0.001 as illustrated in Fig. 4.

An alternate mode of expression of the data in Fig. 3 is to plot the Gaussian dispersion parameter $\sigma/\langle x^2\rangle^{\frac{1}{2}} = \sigma/\sqrt{\sigma^2+\delta^2}$ versus the inverse temperature. This plot is shown in Fig. 5. In line with the extrapolations in Fig. 4, we find here that at the critical point, the Gaussian parameter $\sigma \approx 0.222 \pm 0.001$. Again, as in figure 3, the values in the high temperature region are rising monotonically with L and are below the high temperature fixed point limit. In Fig. 6 we show the behavior of the other Gaussian parameter, $\delta/\sqrt{\sigma^2+\delta^2}$. It tends to a limit of about 0.975 ± 0.001 at $K =$

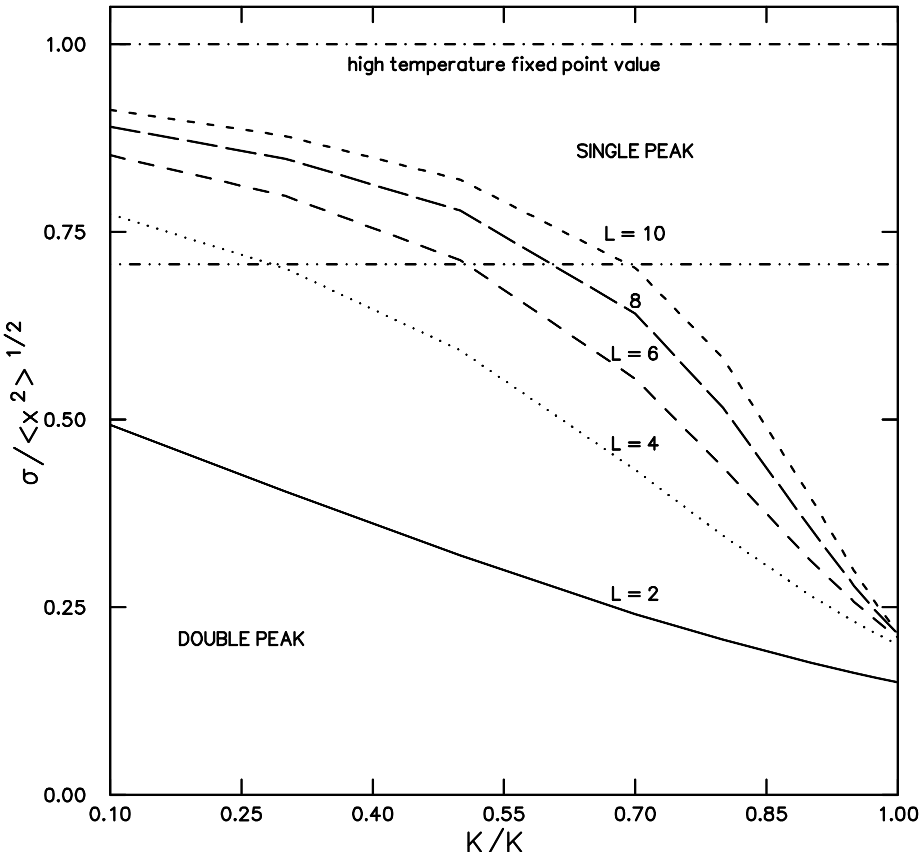

Fig. 5. The the Gaussian parameter σ as a fraction of the root mean square spin. It is plotted against the inverse temperature. For values above $1/\sqrt{2}$, the distribution has a single peak centered at zero. For values less than $1/\sqrt{2}$, there are two peaks, symmetrically situated about zero.

K_c. We know rigorously, as remarked above, that in the limit of infinite block size that $\delta \to 0$ in the high temperature region.

We observe that at the critical point, the mean block-spin is on a scale of $L^{\frac{7}{8}}$ which is intermediate between the scale of $L^{\frac{1}{2}}$ in the high temperature region and the scale of L in the low-temperature region. The block-spin dispersion is about 23% of its length. Thus Kadanoff's idea was roughly right, but since we know that the scale of the block spins is only $L^{\frac{7}{8}}$ and not L, there must be a scattering of overturned spins intrinsic to the block

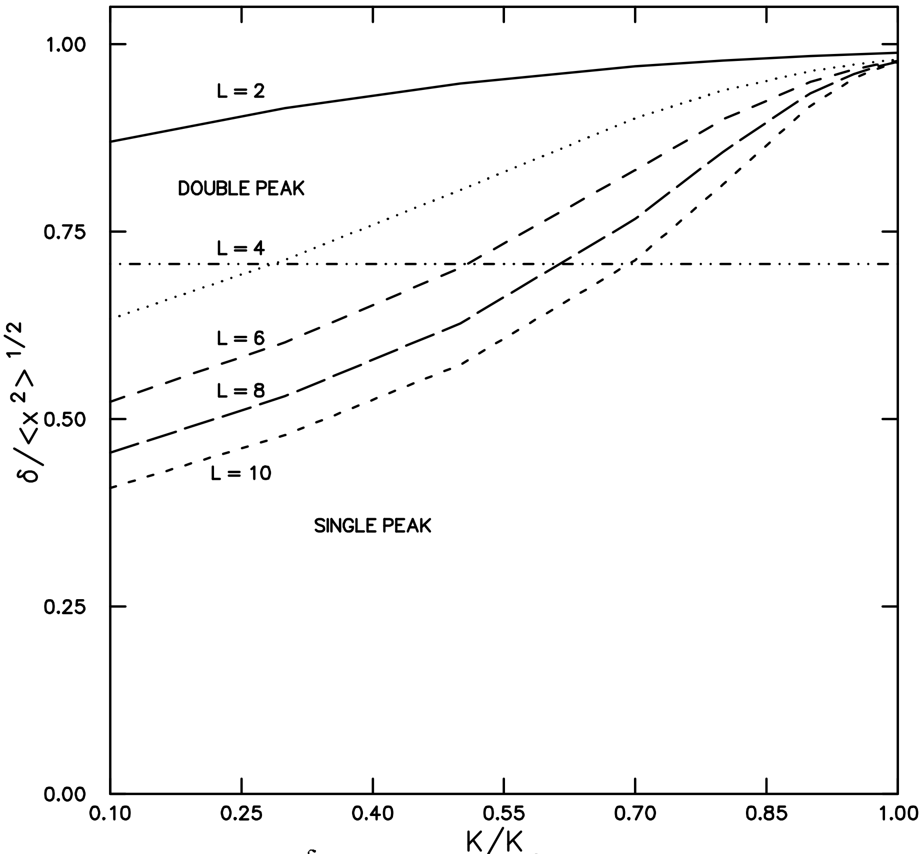

Fig. 6. The the Gaussian parameter δ as a fraction of the root mean square spin. It is plotted against the inverse temperature. For values below $1/\sqrt{2}$, the distribution has a single peak centered at zero. For values above $1/\sqrt{2}$, there are two peaks, symmetrically situated about zero.

description to correct the scale, and hence it seems natural that there also be a dispersion. Therefore we should, a bit more accurately, think of the block spin as having a distributed length.

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